Comp Phys problem set 1

1. Taylor Series / Roundoff errors fight against each other when deciding how long a step function to use when taking derivatives

We're evaluating a function f at 4 points

$$x \pm \delta \quad \& \quad x \pm 2\delta$$

a) estimate of first derivative at x?
   * how can we combine derivative from $x \pm \delta$ with $x \pm 2\delta$ to cancel stuff out of the taylor series?

this is like using the 5 point stencil
$\{x-2\delta, x-\delta, x+\delta, x+2\delta\}$

we can write out the Taylor series of
① $f(x \pm \delta)$ & ② $f(x \pm 2\delta)$

① $$f(x \pm \delta) = f(x) \pm f'(x)\delta + \frac{f''(x)\delta^2}{2} \pm \frac{f'''(x)\delta^3}{6} + \frac{f^4(x)\delta^4}{24}$$
$$\pm f^5(x)\delta^5/120$$

and $f(x+\delta) - f(x-\delta) = 2\delta f'(x) + \frac{f'''(x)\delta^3}{3} + \frac{f^5(x)\delta^5}{60}$

② $f(x \pm 2\delta) = f(x) \pm 2f'(x)\delta + 2f''(x)\delta^2 \pm \frac{4}{3}f'''(x)\delta^3 + \frac{2}{3}f^4(x)\delta^4 \pm \frac{4}{15}f^{(5)}(x)\delta^5$

and $f(x+2\delta) - f(x-2\delta) = 4f'(x)\delta + \frac{8}{3}f'''(x)\delta^3 + \frac{8}{15}f^5(x)\delta^5$

we can take $(8 \cdot ①) - ②$ to cancel out the third order terms in our expressions!

$8 \cdot ① = 16\delta f'(x) + \frac{8f'''}{3}\delta^3 + 8\frac{f^5(x)\delta^5}{60}$

$(8 \cdot ①) - ② = \left(16\delta f'(x) + \cancel{\frac{8}{3}f'''(x)\delta^3} + \frac{2}{15}f^5(x)\delta^5\right) - \left(4\delta f'(x) + \cancel{\frac{8}{3}f'''(x)\delta^3} + \frac{8}{15}f^5(x)\delta^5\right)$

$= 12\delta f'(x) - \frac{6}{15}f^5(x)\delta^5$

$\Rightarrow 8 \cdot f(x+\delta) - 8f(x-\delta) - f(x+2\delta) + f(x-2\delta) = 12\delta f'(x) - \frac{6}{15}\delta^5 f^5(x)$

error term!

$$\left\{ \frac{8f(x+\delta) - 8f(x-\delta) - f(x+2\delta) + f(x-2\delta)}{12\delta} = f'(x) - \frac{1}{30}\delta^4 f^5(x) \right\}$$

b) What should δ be in terms of machine precision & various properties of the function?

We want to find the optimal δ. We know that

$$\bar{f}(x) = f(x) + \varepsilon f(x)$$

, where $\bar{f}(x)$ is what the computer will find

meaning $\bar{f}(x) - f(x) = \varepsilon f(x)$. This makes sense!

we can use our result from a) to find $f'(x) - \bar{f}'(x)$

$$f'(x) - \left[\frac{8(\bar{f}(x+\delta) - 8\bar{f}(x-\delta) - \bar{f}(x+2\delta) + \bar{f}(x-2\delta)}{12\delta}\right].$$

$$f'(x) - \left[\frac{8(fx+\delta) - 8f(x-\delta) - f(x+2\delta) + f(x-2\delta)}{12\delta}\right]$$

→ error term from a)!

$$+ \left[\frac{8\varepsilon f(x+\delta) - 8\varepsilon f(x-\delta) - \varepsilon f(x+2\delta) + \varepsilon f(x-2\delta)}{12\delta}\right]$$

depends on computer precision

→ Floating point noise!

$$\frac{\delta^4}{30} f^5(x) + \frac{18}{12\delta} \varepsilon f(x)$$

to optimize δ we differentiate with respect to δ and equate to 0

$$\frac{4\delta^3}{30} f^5(x) + \frac{18}{12} \varepsilon \cdot \left(-\frac{1}{\delta^2}\right) f(x) = 0$$

$$\frac{2}{15} \delta^3 f^5(x) = \frac{3}{2} \frac{\varepsilon}{\delta^2} \cdot f(x)$$

$$\delta^5 = \frac{45 \varepsilon f(x)}{4 f^5(x)}$$

$$\left\{ \delta = \left[\frac{45 \varepsilon}{4} \frac{f(x)}{f^5(x)} \right]^{1/5} \right\}$$

We can now check this for $f(x) = e^x$ and
$f(x) = e^{0.01x}$